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The Kohn-Hulthén Variational Procedure for the Scattering Operator and the Reactance Operator

Part I: Elementary Form of the Variational Principles

HARRY E. MOSES

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Part I: Elementary Form of the Variational Principles

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Abstract

It is shown how the Kohn-Hulthén variational procedure may be used to approximate both the scattering operator and the reactance operator in terms of an abstract formalism. The procedure for obtaining these operators is then given explicitly for the radial equation ($\ell = 0$), and one- and three-dimensional scattering problems, and the problem of the scattering of an electron by a heavy atom.

1. Introduction

The Kohn-Hulthén variational principle has previously been set up for determining the phase of the solution of the radial equation and for determining the amplitude of the scattered wave in the three-dimensional scattering problem (Kohn[1]). Later the Kohn-Hulthén variational procedure for obtaining the scattering operator was derived as a generalization of the latter procedure (Moses[2]). In the present paper we shall introduce the variational procedure for the reactance operator (cf. Lippmann and Schwinger[3]). The advantage of such a procedure is that a reactance operator so calculated, even though approximate, will be Hermitian for any trial function. Hence the scattering operator which will be calculated through the use of such an approximate reactance operator will be unitary.

It will be shown that the variational procedure for the reactance operator is a generalization of Kohn's procedure for determining scattering phases from the radial equation.

Although the variational principle for the scattering operator has already been given in [2], we shall repeat it below in order to contrast it with the variational principle for the reactance operator.

We shall prove the variational principles abstractly. However, to make them more understandable, we shall introduce the $\underset{\sim}{x}$-representation in the next section.

We shall then illustrate these variational principles in terms of the radial equation corresponding to zero angular momentum, the one-dimensional scattering problem, the three-dimensional scattering problem, and the problem of the scattering of the electron by an atom. Because of the possible utility of the examples, we shall present them before giving the proof of the variational character of the principles. In the special cases below the examples can also be proved directly by the method of integrating by parts and using asymptotic forms in the manner of [1].

2. The $\underset{\sim}{x}$-representation

Let H_0 be a Hamiltonian which has a purely continuous spectrum extending from some finite lower limit to infinity. Let $H = H_0 + V$ be a Hamiltonian which has the same continuous spectrum as H_0 and possible point eigenvalues below the continuous spectrum. Further, let us denote by $|E,a>_0$ the eigenstate of H_0 corresponding to the eigenvalue E. These eigenstates are to satisfy the normalization requirement ${}_0<E,a|E',a'>_0 = \delta(E-E')\delta_{aa'}$. The variable a describes the degeneracy. Similarly, let $|E,a>$ be an eigenstate of H corresponding to the eigenvalues E of the continuous spectrum. The eigenvectors $|E, a>$ are not unique. Three separate sets will interest us. They are the " outgoing eigenfunctions" , denoted by $|E,a>_-$, the "incoming eigenfunctions" $|E,a>_+$, and the " standing wave eigenfunctions" $|E,a>_s$. (In the more conventional notation the outgoing eigenfunctions are denoted by a plus subscript and the incoming ones by a minus subscript. We reverse the subscripts to indicate that $|E,a>_-$ and $|E,a>_+$ can be considered to have been obtained from a time-dependent procedure with initial conditions at $t = -\infty$ or final conditions at $t = +\infty$ respectively.)

It will also be convenient to introduce to the symbols $\Psi_0(\underset{\sim}{x}|E,a)$, $\Psi_-(\underset{\sim}{x}|E,a)$, $\Psi_+(\underset{\sim}{x}|E,a)$, $\Psi_s(\underset{\sim}{x}|E,a)$, for $<\underset{\sim}{x}|E,a>_0$, $<\underset{\sim}{x}|E,a>_-$, $<\underset{\sim}{x}|E,a>_s$ respectively. By virtue of the normalization conditions of $|E,a>_0$ we have

$$\int \Psi_0^*(\underset{\sim}{x}|E,a)\Psi_0(\underset{\sim}{x}|E',a')d\underset{\sim}{x} = \delta(E-E')\delta_{aa'} .$$

The eigenstates $|E,a>_\pm$ and $|E,a>_s$ are characterized by the following integral equations:

$$\Psi_-(\underset{\sim}{x}|E,a) = \Psi_0(\underset{\sim}{x}|E,a) + \int G_E^{out}(\underset{\sim}{x}|\underset{\sim}{x}')V(\underset{\sim}{x}')\ \Psi_0(\underset{\sim}{x}'|E,a)\ d\underset{\sim}{x}' \tag{2.1}$$

$$\Psi_+(\underset{\sim}{x}|E,a) = \Psi_0(\underset{\sim}{x}|E,a) + \int G_E^{in}(\underset{\sim}{x}|\underset{\sim}{x}')V(\underset{\sim}{x}')\ \Psi_-(\underset{\sim}{x}'|E,a)\ d\underset{\sim}{x}' \tag{2.2}$$

$$\Psi_s(\underset{\sim}{x}|E,a) = \Psi_0(\underset{\sim}{x}|E,a) + \int G_E^{s}(\underset{\sim}{x}|\underset{\sim}{x}')V(\underset{\sim}{x}')\ \Psi_s(\underset{\sim}{x}'|E,a)d\underset{\sim}{x}' , \tag{2.3}$$

where G_E^{out}, G_E^{in} are the usual outgoing and incoming Green's functions with respect to H_0, and

$$G_E^s(\underset{\sim}{x}|\underset{\sim}{x}') = \frac{1}{2}\left[G_E^{out}(\underset{\sim}{x}|\underset{\sim}{x}') + G_E^{in}(\underset{\sim}{x}|\underset{\sim}{x}')\right].$$

It is to be noted that $G_E^s(\underset{\sim}{x}|\underset{\sim}{x}')$ is Hermitian, i.e., $G_E^s(\underset{\sim}{x}|\underset{\sim}{x}') = G_E^s(\underset{\sim}{x}'|\underset{\sim}{x})^*$. Explicitly

$$(2.4a) \qquad G_E^{out}(\underset{\sim}{x}|\underset{\sim}{x}') = \iint \Psi_0^*(\underset{\sim}{x}|E',a')\gamma_-(E-E')\Psi_0(\underset{\sim}{x}'|E',a')dE'da',$$

$$(2.4b) \qquad G_E^{in}(\underset{\sim}{x}|\underset{\sim}{x}') = \iint \Psi_0^*(\underset{\sim}{x}|E',a')\gamma_+(E-E')\Psi_0(\underset{\sim}{x}'|E',a')dE'da',$$

$$(2.4c) \qquad G_E^s(\underset{\sim}{x}|\underset{\sim}{x}') = \iint \Psi_0^*(\underset{\sim}{x}|E',a')\,\frac{P}{E-E'}\,\Psi_0(x'|E',a')dE'da',$$

where

$$(2.4d) \qquad \gamma_\pm(x) = \pm i\pi\,\delta(x) + \frac{P}{x} = \lim_{\varepsilon \to \mp 0} \frac{1}{x+i\varepsilon}$$

and the symbol P means that in integrations, the Cauchy principal part of the integral is to be taken. The scattering operator S and its inverse S^{-1} as given in the H_0-representation has the form

$$(2.5) \qquad \begin{aligned} {}_0\langle E,a|S|E',a'\rangle_0 &= \delta(E-E')\left[\delta_{aa'} - 2\pi i\;{}_0\langle E,a|T_-|E,a'\rangle_0\right], \\ {}_0\langle E,a|S^{-1}|E',a'\rangle_0 &= \delta(E-E')\left[\delta_{aa'} + 2\pi i\;{}_0\langle E,a|T_+|E,a'\rangle_0\right] \end{aligned}$$

where $\delta_{aa'}$ is a suitably generalized δ-function and $T_\pm$ are operators given by

$$(2.6) \qquad \begin{aligned} {}_0\langle E,a|T_\pm|E',a'\rangle_0 &= {}_0\langle E,a|V|E',a'\rangle_\pm \\ &= \int \Psi_0^*(\underset{\sim}{x}|E,a)\;V(\underset{\sim}{x})\;\Psi_\pm(\underset{\sim}{x}|E',a')d\underset{\sim}{x}\,. \end{aligned}$$

The quantity ${}_0\langle E,a|T_\pm|E,a'\rangle_0$ is essentially the amplitude of the scattered wave in the domain where $V(\underset{\sim}{x})$ is small when the appropriate coordinate in $\Psi_s(\underset{\sim}{x}|E,a)$ is taken to be infinity.

We define the reactance operator K in the customary way by

$$S = \left[I - i\pi K \right] \left[I + i\pi K \right]^{-1} . \tag{2.7}$$

K can be shown to be Hermitian. In terms of the H_0 representation, K is given by

$$_0\!< E,a|K|E',a' >_0 \;=\; \delta(E-E')\; _0\!< E,a|T_s|E,a' >_s , \tag{2.8}$$

where

$$_0\!< E,a|T_s|E',a' >_0 = \;_0\!< E,a|V|E',a' >_s = \int \Psi_0^*(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})\Psi_s(\underset{\sim}{x}|E',a')d\underset{\sim}{x} . \tag{2.9}$$

From (2.5) and (2.7) it can be shown that

$$_0\!< E,a|T_-|E,a' >_0 \;=\; \sum_{a''}\; _0\!< E,a|T_s|E,a'' >_0 \;_0\!< E,a''|C|E,a' >_0 , \tag{2.10}$$

where $_0\!< E,a|C|E,a' >_0$ is the inverse of $\left[\delta_{aa'} + i\pi\; _0\!< E,a|T_s|E,a' >_0\right]$ insofar as these quantities are matrices (or integral operators) in the variables a, a'; that is,

$$\begin{aligned} &\sum_{a''}\; _0\!< E,a|C|E,a'' >_0 \left[\delta_{a''a'} + i\pi\; _0\!< E,a''|T_s|E,a' >_0\right] \\ &= \sum_{a''}\left[\delta_{aa''} + i\pi\; _0\!< E,a|T_s|E,a'' >_0\right] {}_0\!< E,a''|C|E,a' >_0 \;=\; \delta_{aa'} . \end{aligned} \tag{2.11}$$

The quantity $_0\!< E,a|T_s|E,a' >_0$ can be shown to be the amplitude of scattered waves in the asymptotic form of $\Psi_s(\underset{\sim}{x}|E,a)$.

There are two variational principles of the Kohn-Hulthén type. One is used to approximate $_0\!< E,a|T_-|E,a' >_0$ directly. The second is used to approximate $_0\!< E,a|T_s|E,a' >_0$, from which $_0\!< E,a|T_-|E,a' >_0$ can be obtained by means of (2.10) and (2.11). The advantage of the latter procedure is that the scattering matrix so obtained will be unitary because the approximate elements

${}_0\langle E,a|T_s|E,a'\rangle_0$ will correspond to a Hermitian reactance operator for any trial function. However, it should be noted that to solve (2.11) for ${}_0\langle E,a|C|E,a'\rangle_0$ is, in general, difficult if the degeneracy variables can take on an infinite number of values.

In the case of the variational principle for ${}_0\langle E,a|T_-|E,a'\rangle_0$, we have generally

$$
\begin{aligned}
{}_0\langle E,a|T_-|E,a'\rangle_0 \cong \lim_{\nu\to 0} \int \Psi^*_{+t}(\underset{\sim}{x}|E+\nu,a)\left[H^{\underset{\sim}{x}} - E\right]\Psi_{-t}(\underset{\sim}{x}|E,a')\,dx& \\
(2.12) \qquad + {}_0\langle E,a|T_{-t}|E,a'\rangle_0 \,.&
\end{aligned}
$$

In (2.12), $H^{\underset{\sim}{x}}$ represents the total Hamiltonian as given in the $\underset{\sim}{x}$-representation, and the quantity ${}_0\langle E,a|T_{-t}|E,a'\rangle_0$ is a "trial function" which approximates ${}_0\langle E,a|T_-|E,a'\rangle_0$. Furthermore, $\Psi_{-t}(\underset{\sim}{x}|E,a)$ is a function which approximates the exact eigenfunction $\Psi_-(\underset{\sim}{x}|E,a)$: $\Psi_{-t}(\underset{\sim}{x}|E,a)$ is required to have the same asymptotic form as $\Psi_-(\underset{\sim}{x}|E,a)$, except that the amplitude of the scattered wave ${}_0\langle E,a|T_-|E,a'\rangle_0$ is replaced by ${}_0\langle E,a|T_{-t}|E,a'\rangle_0$. Likewise $\Psi_{+t}(\underset{\sim}{x}|E,a)$ approximates the exact eigenfunction $\Psi_+(\underset{\sim}{x}|E,a)$ and satisfies the same type of asymptotic boundary condition, except that the exact amplitude ${}_0\langle E,a|T_+|E,a'\rangle_0$ is replaced by the trial amplitude ${}_0\langle E,a|T_{+t}|E,a'\rangle_0$.

The limit $\lim_{\nu\to 0}$ is introduced to prevent an ambiguity in the definition of the integral. This point is discussed more fully in [2].

The variational principle (2.12) can be written in another form. The boundary conditions on $\Psi_{\pm t}(\underset{\sim}{x}|E,a)$ imply that there exist functions $\phi_{\pm t}(\underset{\sim}{x}|E,a)$ which satisfy

$$
(2.13) \qquad \Psi_{\pm t}(\underset{\sim}{x}|E,a) = \Psi_0(\underset{\sim}{x}|E,a) + \int G_E^{\substack{\mathrm{in}\\ \mathrm{out}}}(\underset{\sim}{x}|\underset{\sim}{x}')\,\phi_{\pm t}(\underset{\sim}{x}'|E,a)\,d\underset{\sim}{x}' .
$$

In fact, one may regard $\phi_{\pm t}(\underset{\sim}{x}|E,a)$ as the true trial functions. Then $\Psi_{\pm t}(\underset{\sim}{x}|E,a)$ will automatically satisfy the boundary conditions, provided one picks

${}_0\langle E,a|T_{-t}|E,a'\rangle_0$ to be the amplitude of the scattered wave associated with $\Psi_{-t}(\underset{\sim}{x}|E,a)$. We can express the variational principle in terms of essentially arbitrary $\phi_{\pm t}(\underset{\sim}{x}|E,a)$ without indicating boundary conditions:

$$
\begin{aligned}
(2.14)\qquad {}_0\langle E,a|T_-|E,a'\rangle_0 \cong \int & \Psi_0^*(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})\Psi_0(E,a')d\underset{\sim}{x} \\
&+ \iint \Psi_0^*(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})G_E^{\text{out}}(\underset{\sim}{x}|\underset{\sim}{x}')V(\underset{\sim}{x}')\phi_{-t}(\underset{\sim}{x}'|E,a')d\underset{\sim}{x}d\underset{\sim}{x}' \\
&+ \iint \phi_{+t}^*(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})G_E^{\text{out}}(\underset{\sim}{x}|\underset{\sim}{x}')V(\underset{\sim}{x}')\Psi_0(\underset{\sim}{x}'|E,a')d\underset{\sim}{x}d\underset{\sim}{x}' \\
&- \iint \phi_{+t}^*(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})G_E^{\text{out}}(\underset{\sim}{x}|\underset{\sim}{x}')V(\underset{\sim}{x}')\phi_{-t}(\underset{\sim}{x}'|E,a')d\underset{\sim}{x}d\underset{\sim}{x}' \\
&+ \iiint \phi_{+t}^*(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})G_E^{\text{out}}(\underset{\sim}{x}|\underset{\sim}{x}')V(\underset{\sim}{x}')G_E^{\text{out}}(\underset{\sim}{x}'|\underset{\sim}{x}'') \\
&\qquad\qquad V(\underset{\sim}{x}'')\phi_{-t}(\underset{\sim}{x}''|E,a')d\underset{\sim}{x}d\underset{\sim}{x}'d\underset{\sim}{x}'' .
\end{aligned}
$$

The forms (2.12) and (2.14) are entirely equivalent. The form (2.12) has the disadvantage that the trial functions $\Psi_{\pm t}(\underset{\sim}{x}|E,a)$ are required to satisfy restrictive boundary conditions. However, it has the advantage in that the Green's function does not appear explicitly. Conversely, the advantage of the form (2.14) is that we may pick $\phi_{\pm t}(\underset{\sim}{x}|E,a)$ in an essentially arbitrary fashion; and, the disadvantage of this form is that the Green's function appears explicitly in the integral.

We shall now write the corresponding variational principles for ${}_0\langle E,a|T_s|E,a'\rangle_0$. The analogue to (2.12) is

$$
(2.15)\qquad {}_0\langle E,a|T_s|E,a'\rangle_0 \cong \lim_{\nu\to 0}\int \Psi_{st}^*(\underset{\sim}{x}|E+\nu,a)\left[H^{\underset{\sim}{x}}-E\right]\Psi_{st}(\underset{\sim}{x}|E,a')d\underset{\sim}{x} + {}_0\langle E,a|T_{st}|E,a'\rangle_0 ,
$$

where ${}_0\langle E,a|T_{st}|E,a'\rangle_0$ is a trial function for ${}_0\langle E,a|T_s|E,a'\rangle_0$. The function $\Psi_{st}(\underset{\sim}{x}|E,a')$ approximates the function $\Psi_s(\underset{\sim}{x}|E,a')$ in the sense that the former satisfies the same boundary conditions as the latter, except that the amplitude ${}_0\langle E,a|T_s|E,a'\rangle_0$ of the asymptotic form of Ψ_s is replaced by ${}_0\langle E,a|T_{st}|E,a'\rangle_0$.

The analogue of (2.14) is

$$
\begin{aligned}
{}_0\langle E,a|T_s|E,a'\rangle_0 \cong & \int \Psi_0^*(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})\Psi_0(\underset{\sim}{x}|E,a')d\underset{\sim}{x} \\
& + \iint \Psi_0^*(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})G_E^s(\underset{\sim}{x}|\underset{\sim}{x}')V(\underset{\sim}{x}')\phi_{st}(\underset{\sim}{x}'|E,a')d\underset{\sim}{x}d\underset{\sim}{x}' \\
& + \iint \phi_{st}^*(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})G_E^s(\underset{\sim}{x}|\underset{\sim}{x}')V(\underset{\sim}{x}')\Psi_0(\underset{\sim}{x}|E,a')d\underset{\sim}{x}d\underset{\sim}{x}' \\
& - \iint \phi_{st}^*(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})G_E^s(\underset{\sim}{x}|\underset{\sim}{x}')V(\underset{\sim}{x}')\phi_{st}(\underset{\sim}{x}'|E,a')d\underset{\sim}{x}d\underset{\sim}{x}' \\
& + \iiint \phi_{st}^*(\underset{\sim}{x}|E,a)V(\underset{\sim}{x})G_E^s(\underset{\sim}{x}|\underset{\sim}{x}')V(\underset{\sim}{x}')G_E^s(\underset{\sim}{x}'|\underset{\sim}{x}'')V(\underset{\sim}{x}'')\phi_{st}(\underset{\sim}{x}''|E,a') \\
& \qquad\qquad d\underset{\sim}{x}d\underset{\sim}{x}'d\underset{\sim}{x}'' ,
\end{aligned}
\tag{2.16}
$$

which is obtained from (2.15) by writing

$$
\Psi_{st}(\underset{\sim}{x}|E,a) = \Psi_0(\underset{\sim}{x}|E,a) + \int G_E^s(\underset{\sim}{x}|\underset{\sim}{x}')V(\underset{\sim}{x}')\phi_{st}(\underset{\sim}{x}'|E,a)dx' . \tag{2.16a}
$$

Equation (2.16) shows that the approximate value of ${}_0\langle E,a|T_s|E,a'\rangle_0$ is Hermitian in the variables a, a' for any trial function Ψ_{st} that satisfies the appropriate boundary conditions.

We shall now specialize the results to the examples mentioned in the Introduction. Instead of expressing the various eigenfunctions in terms of the energy eigenvalue E and degeneracy variable a, we shall express these eigenfunctions in terms of the momentum representation as is conventional. These two sets of eigenfunctions differ only by a Jacobian of the transformation between the sets of variables. However, for consistency, we shall adhere to our original definitions of ${}_0\langle E,a|T_\pm|E,a'\rangle_0$ and ${}_0\langle E,a|T_s|E,a'\rangle_0$ (see (2.6) and (2.9)) which are given in terms of energy eigenvalues and degeneracy variables. In some cases the Jacobian of the transformation (a known function) will appear in a somewhat clumsy form. We shall only indicate the principles (2.12) and (2.15) in which the Green's functions do not appear explicitly. The principles (2.14) and (2.16) can be obtained similarly,

3. The radial equation for zero angular momentum

As the sole variable in the coordinate representation we take r in the range $0 \leq r < \infty$. All states f(r) are to satisfy

$$(3.1) \qquad f(0) = 0.$$

In particular, the eigenstates of H_o and H must satisfy this requirement. The operators H_o and H are given by

$$(3.2) \qquad H_o = -\frac{d^2}{dr^2}$$

$$(3.3) \qquad H = -\frac{d^2}{dr^2} + V(r) .$$

The normalized eigenfunctions of H_o corresponding to the eigenvalue $k^2 = E$ are

$$(3.4) \qquad \Psi_o(r|k) = \sqrt{\frac{2}{\pi}} \sin kr, \qquad (k > 0).$$

The Green's functions G_E^{in}, G_E^{out}, G_E^s are given by

$$(3.5) \qquad G_E^{out}(r|r') = -\frac{1}{k}\left\{\eta(r-r')e^{ikr}\sin kr' + \eta(r'-r)e^{ikr'}\sin kr\right\},$$

$$(3.6) \qquad G_E^{in}(r|r') = -\frac{1}{k}\left\{\eta(r-r')e^{-ikr}\sin kr' + \eta(r'-r)e^{-ikr'}\sin kr\right\},$$

$$(3.7) \qquad G_E^{s}(r|r') = -\frac{1}{k}\left\{\eta(r-r')\cos kr \sin kr' + \eta(r'-r)\cos kr' \sin kr\right\}.$$

The function $\eta(x)$ is the Heaviside step function defined by

$$(3.8) \qquad \begin{aligned} \eta(x) &= 1, \quad x > 0 \\ &= 0, \quad x < 0. \end{aligned}$$

The eigenfunctions of H which are relevant are given by

$$(3.9) \qquad \Psi_{\pm}(r|k) = \sqrt{\frac{2}{\pi}}\,\sin kr - \frac{1}{k}\,e^{\mp ikr}\int_0^r \sin kr'\,V(r')\Psi_{\pm}(r'|k)dr' - \frac{1}{k}\sin kr\int_r^{\infty} e^{\mp ikr'}\,V(r')\Psi_{\pm}(r'|k)dr' ,$$

$$(3.10) \qquad \Psi_{s}(r|k) = \sqrt{\frac{2}{\pi}}\,\sin kr - \frac{1}{k}\cos kr\int_0^r \sin kr'\,V(r')\Psi_{s}(r'|k)dr' - \frac{1}{k}\sin kr\int_r^{\infty} \cos kr'\,V(r')\Psi_{s}(r'|k)dr' .$$

Since there is no degeneracy, the variable a will play no role.

The quantities ${}_{0}\langle E|T_{\pm}|E\rangle_{0}$ and ${}_{0}\langle E|T_{s}|E\rangle_{0}$ can be obtained from the asymptotic forms of $\Psi_{\pm}$ and Ψ_{s} respectively. One can easily show that

$$(3.11) \qquad \lim_{r\to\infty}\Psi_{\pm}(r|k) = \sqrt{\frac{2}{\pi}}\,\sin kr - \sqrt{2\pi}\;e^{\mp ikr}\;{}_{0}\langle E|T_{\pm}|E\rangle_{0} ,$$

$$(3.12) \qquad \lim_{r\to\infty}\Psi_{s}(r|k) = \sqrt{\frac{2}{\pi}}\,\sin kr - \sqrt{2\pi}\,\cos kr\;{}_{0}\langle E|T_{s}|E\rangle_{0} .$$

If one writes (3.12) in the form where the phase shift appears explicitly, i.e.,

$$(3.12a) \qquad \lim_{r\to\infty}\Psi_{s}(r|k) \to A\sin(kr+\phi),$$

then from (3.12) one sees (cf. [3])

$$(3.12b) \qquad A = \sqrt{\frac{2}{\pi}}\,\left(1+\pi^{2}\,{}_{0}\langle E|T_{s}|E\rangle_{0}^{2}\right)^{1/2} = \sqrt{\frac{2}{\pi}}\,\sec\phi,$$

$$\tan\phi = -\pi\;{}_{0}\langle E|T_{s}|E\rangle_{0} .$$

The Kohn-Hulthén variational principle was originally set up for tan ϕ and hence for ${}_{0}\langle E|T_{s}|E\rangle_{0}$, which is essentially the reactance operator for the radial equation.

The variational principle for the scattering operator is

$$ {}_o\langle E|T_-|E\rangle_o \cong \lim_{k'\to k} \frac{1}{2k} \int \Psi^*_{+t}(r|k')\left[-\frac{d^2}{dr^2} + V(r) - k^2\right]\Psi_{-t}(r|k)dr + {}_o\langle E|T_{-t}|E\rangle_o, \tag{3.13} $$

where ${}_o\langle E|T_{-t}|E\rangle_o$ is an approximation to ${}_o\langle E|T_-|E\rangle_o$ and $\Psi_{\pm t}$ are trial functions which have the asymptotic form (3.11) with ${}_o\langle E|T_\pm|E\rangle_o$ replaced by ${}_o\langle E|T_{\pm t}|E\rangle_o$. As before, we take $E = k^2$, $k > 0$.

The variational principle for the reactance operator is

$$ {}_o\langle E|T_s|E\rangle_o \cong \lim_{k'\to k} \frac{1}{2k} \int \Psi^*_{st}(r|k')\left[-\frac{d^2}{dr^2} + V(r) - k^2\right]\Psi_{st}(r|k)dr + {}_o\langle E|T_{st}|E\rangle_o, \tag{3.14} $$

where Ψ_{st} has the same asymptotic form as (3.12) with ${}_o\langle E|T_s|E\rangle_o$ replaced by the trial function ${}_o\langle E|T_{st}|E\rangle_o$.

4. The one-dimensional scattering problem

In one dimension the variable x has the range $-\infty < x < \infty$. H and H_o are given by

$$ H_o = -\frac{d}{dx^2} \tag{4.1} $$

$$ H = -\frac{d}{dx^2} + V(x). \tag{4.2} $$

The eigenfunctions of H_o are

$$ \Psi_o(x|k) = \frac{1}{\sqrt{2\pi}}\, e^{ikx} \qquad (-\infty < k < \infty) \tag{4.3} $$

and the pertinent Green's functions are

$$(4.4)\qquad G_E^{out}(x|x') = -\frac{i}{2|k|}\, e^{i|k||x-x'|},$$

$$(4.5)\qquad G_E^{in}(x|x') = \frac{i}{2|k|}\, e^{-i|k||x-x'|},$$

$$(4.6)\qquad G_E^{s}(x|x') = \frac{1}{2|k|}\sin|k||x-x'|,$$

In (4.4)-(4.6), E is given by $E = k^2$. The appropriate eigenfunctions of H satisfy the integral equations

$$(4.7)\qquad \Psi_o(x|k) = \frac{1}{\sqrt{2\pi}}\, e^{ikx},$$

$$(4.8)\qquad \Psi_\pm(x|k) = \frac{1}{\sqrt{2\pi}}\, e^{ikx} \pm \frac{i}{2|k|}\int_{-\infty}^{+\infty} e^{\mp i|k||x-x'|}V(x')\Psi_\pm(x'|k)\,dx',$$

$$(4.9)\qquad \Psi_s(x|k) = \frac{1}{\sqrt{2\pi}}\, e^{ikx} + \frac{1}{2|k|}\int_{-\infty}^{+\infty} \sin|k||x-x'|\,V(x')\Psi_s(x'|k)\,dx'.$$

We can show that ${}_o\langle E,a|T_\pm|E,a'\rangle_o$ is essentially the amplitude of the scattered wave arising in $\Psi_\pm(x|k)$ when $|x| \to \infty$. We have, in fact,

$$(4.10)\qquad \lim_{|x|\to\infty} \Psi_\pm(x|k) = \frac{1}{\sqrt{2\pi}}\, e^{ikx} \pm \sqrt{2\pi}\, i\, e^{\mp i|k||x|}\,{}_o\langle E,\mp b|T_\pm|E,a\rangle_o$$

where

$$(4.10a)\qquad E = k^2, \qquad a = \frac{k}{|k|}, \qquad b = \frac{x}{|x|}\ .$$

In (4.10) the top signs and bottom signs are taken together. The degeneracy variables a, b can thus take on only the values of ± 1. It can also be shown that

$$(4.11)\qquad \lim_{|x|\to\infty} \Psi_s(x|k) = \frac{e^{ikx}}{\sqrt{2\pi}} - \sqrt{\frac{\pi}{2}}\, i \left\{ e^{i|k||x|}\ {}_o\langle E,b|T_s|E,a\rangle_o - e^{-i|k||x|}\ {}_o\langle E,-b|T_s|E,a\rangle_o \right\},$$

where a and b are defined in (4.10a).

The variational principle for ${}_o\langle E,a|T_-|E,b\rangle_o$ is then

$$(4.12)\qquad {}_o\langle E,a|T_-|E,b\rangle_o \cong \frac{1}{2|k|} \lim_{|k'|\to|k|} \int \Psi^*_{+t}(x|k')\left[-\frac{d^2}{dx^2} + V(x)-k^2\right] \cdot \Psi_{-t}(x|k)\, dx + {}_o\langle E,a|T_{-t}|E,b\rangle_o ,$$

where ${}_o\langle E,a|T_{-t}|E,b\rangle_o$ is the trial function for ${}_o\langle E,a|T_-|E,b\rangle$ and $\Psi_{-t}(x|k)$ and $\Psi_{+t}(x|k')$ are trial functions which have the asymptotic form (4.10) with the amplitude ${}_o\langle E,a|T_\pm|E,b\rangle$ replaced by the trial amplitudes $\langle E,a|T_{\pm t}|E,b\rangle$. In (4.12)

$$(4.12a)\qquad E = k^2, \qquad a = \frac{k'}{|k'|}, \qquad b = \frac{k}{|k|} .$$

The variational principle for ${}_o\langle E,a|T_s|E,b\rangle_o$ is

$$(4.13)\qquad {}_o\langle E,a|T_s|E,b\rangle_o = \frac{1}{2|k|} \lim_{|k'|\to|k|} \int \Psi^*_{st}(x|k')\left[-\frac{d^2}{dx^2} + V(x)-k^2\right] \cdot \Psi_{st}(x|k)dx + {}_o\langle E,a|T_{st}|E,b\rangle_o .$$

Again

$$(4.13a)\qquad E = k^2, \qquad a = \frac{k'}{|k'|}, \qquad b = \frac{k}{|k|},$$

and ${}_o\langle E,a|T_{st}|E,b\rangle_o$ is a trial function for ${}_o\langle E,a|T_s|E,b\rangle_o$. The functions $\Psi_{st}(x|k)$ are chosen so as to have the asymptotic form (4.11) with ${}_o\langle E,a|T_s|E,b\rangle_o$

replaced by ${}_{o}\langle E,a|T_{st}|E,b\rangle_{o}$.

5. Three-dimensional scattering problem

In this case H_o and H are given by

$$(5.1)\qquad H_o = -\nabla^2$$

$$(5.2)\qquad H = -\nabla^2 + V(\underset{\sim}{x}) .$$

The eigenfunctions of H_o are

$$(5.3)\qquad \Psi_o(\underset{\sim}{x}|\underset{\sim}{k}) = \frac{1}{(2\pi)^{3/2}}\, e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}}$$

and the appropriate Green's functions are

$$(5.4)\qquad G_E^{out}(\underset{\sim}{x}|\underset{\sim}{x}') = -\frac{1}{4\pi}\,\frac{e^{i|\underset{\sim}{k}||\underset{\sim}{x}-\underset{\sim}{x}'|}}{|\underset{\sim}{x}-\underset{\sim}{x}'|} ,$$

$$(5.5)\qquad G_E^{in}(\underset{\sim}{x}|\underset{\sim}{x}') = -\frac{1}{4\pi}\,\frac{e^{-i|\underset{\sim}{k}||\underset{\sim}{x}-\underset{\sim}{x}'|}}{|\underset{\sim}{x}-\underset{\sim}{x}'|} ,$$

$$(5.6)\qquad G_E^{s}(\underset{\sim}{x}|\underset{\sim}{x}') = -\frac{1}{4\pi}\,\frac{\cos|\underset{\sim}{k}||\underset{\sim}{x}-\underset{\sim}{x}'|}{|\underset{\sim}{x}-\underset{\sim}{x}'|} .$$

In (5.4)-(5.6), $E = |\underset{\sim}{k}|^2$. Again we shall express our results in terms of the momentum representation. The appropriate eigenfunctions in terms of this representation are

$$(5.7)\qquad \Psi_o(\underset{\sim}{x}|\underset{\sim}{k}) = \frac{1}{(2\pi)^{3/2}}\, e^{i(\underset{\sim}{k}\cdot\underset{\sim}{x})} ,$$

$$(5.8)\qquad \Psi_\pm(\underset{\sim}{x}|\underset{\sim}{k}) = \frac{1}{(2\pi)^{3/2}}\, e^{i(\underset{\sim}{k}\cdot\underset{\sim}{x})} - \frac{1}{4\pi}\int \frac{e^{\mp i|\underset{\sim}{k}||\underset{\sim}{x}-\underset{\sim}{x}'|}}{|\underset{\sim}{x}-\underset{\sim}{x}'|}\, V(\underset{\sim}{x}')\Psi_\pm(\underset{\sim}{x}'|\underset{\sim}{k})d\underset{\sim}{x}' ,$$

$$(5.9)\qquad \Psi_s(\underset{\sim}{x}|\underset{\sim}{k}) = \frac{1}{(2\pi)^{3/2}}\, e^{i(\underset{\sim}{k}\cdot\underset{\sim}{x})} - \frac{1}{4\pi}\int \frac{\cos|\underset{\sim}{k}||\underset{\sim}{x}-\underset{\sim}{x}'|}{|\underset{\sim}{x}-\underset{\sim}{x}'|}\, V(\underset{\sim}{x}')\Psi_s(\underset{\sim}{x}'|k)d\underset{\sim}{x}' .$$

The function ${}_0\langle E,a|T_-|E,a'\rangle_0$ can be expressed in terms of the amplitude of the spherical wave obtained by letting $|\underset{\sim}{x}| \to \infty$ in $\Psi_-(\underset{\sim}{x}|\underset{\sim}{k})$:

$$(5.10)\qquad \lim_{|\underset{\sim}{x}|\to\infty} \Psi_-(\underset{\sim}{x}|\underset{\sim}{k}) = \frac{1}{(2\pi)^{3/2}}\, e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}} - \sqrt{2\pi}\, \frac{e^{i|\underset{\sim}{k}||\underset{\sim}{x}|}}{|\underset{\sim}{x}||\underset{\sim}{k}|} (\sin\theta\sin\theta')^{-1/2}\, {}_0\langle E,\theta',\emptyset'|T_-|E,\theta,\emptyset\rangle_0 \;.$$

The variables θ, $\emptyset$ are now the degeneracy variables previously collectively denoted by a. In fact in (3.6) we have

(5.10a) $|\underset{\sim}{k}| = \sqrt{E}$; θ is the angle which $\underset{\sim}{k}$ makes with the z-axis and $\emptyset$ is the angle which the projection of $\underset{\sim}{k}$ in the x-y-plane makes with the x-axis; θ', $\emptyset'$ are the corresponding angles associated with the vector $\underset{\sim}{x}$.

Similarly

$$(5.11)\qquad \lim_{|\underset{\sim}{x}|\to\infty} \Psi_+(\underset{\sim}{x}|\underset{\sim}{k}) = \frac{1}{(2\pi)^{3/2}}\, e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}} - \sqrt{2\pi}\, \frac{e^{-i|\underset{\sim}{k}||\underset{\sim}{x}|}}{|\underset{\sim}{x}||\underset{\sim}{k}|} (\sin\theta\sin\theta')^{-1/2}\, {}_0\langle E,\pi-\theta',\pi+\emptyset'|T_+|E,\theta,\emptyset\rangle_0 \,,$$

$$(5.12)\qquad \lim_{|\underset{\sim}{x}|\to\infty} \Psi_s(\underset{\sim}{x}|\underset{\sim}{k}) = \frac{1}{(2\pi)^{3/2}}\, e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}} - \sqrt{\frac{\pi}{2}}\, \frac{1}{|\underset{\sim}{x}||\underset{\sim}{k}|} (\sin\theta\sin\theta')^{-1/2} \cdot \left\{ {}_0\langle E,\theta',\emptyset'|T_s|E,\theta,\emptyset\rangle_0\, e^{i|\underset{\sim}{k}||\underset{\sim}{x}|} + {}_0\langle E,\pi-\theta',\pi+\emptyset'|T_s|F,\theta,\emptyset\rangle_0\, e^{-i|\underset{\sim}{k}||\underset{\sim}{x}|} \right\} .$$

In (5.11), (5.12) we also use (5.10a). The variational expression for ${}_0\langle E,a|T_-|E,b\rangle_0$ is

$$(5.13)\quad {}_0\langle E,\theta',\phi'|T_-|E,\theta,\phi\rangle_0 \simeq \frac{|\underset{\sim}{k}|}{2}(\sin\theta\sin\theta')^{\frac{1}{2}} \lim_{|\underset{\sim}{k}'|\to|\underset{\sim}{k}|}\left\{\int \Psi^*_{+t}(\underset{\sim}{x}|\underset{\sim}{k}')\cdot\left[-\nabla^2+V(x)-k^2\right]\Psi_{-t}(\underset{\sim}{x}|\underset{\sim}{k})dx\right\} + {}_0\langle E,\theta',\phi'|T_{-t}|E,\theta,\phi\rangle_0 ,$$

where ${}_0\langle E,\theta',\phi'|T_{-t}|E,\theta,\phi\rangle_0$ approximates ${}_0\langle E,\theta',\phi'|T_-|E,\theta,\phi\rangle_0$ and $\Psi_{\pm t}$ have the same asymptotic form as (5.10) and (5.11) for $\Psi_\pm$ with ${}_0\langle E,\theta',\phi'|T_\pm|E,\theta,\phi\rangle_0$ replaced by ${}_0\langle E,\theta',\phi'|T_{\pm t}|E,\theta,\phi\rangle_0$. In (5.13) we have

$$(5.13a)\qquad E = |\underset{\sim}{k}|^2;\quad \theta,\ \phi = \text{polar angles of } \underset{\sim}{k};$$
$$\theta',\phi' = \text{polar angles of } \underset{\sim}{k}'.$$

This variational principle is also given in a somewhat different form in [1]. The variational expression for ${}_0\langle E,a|T_s|E,b\rangle_0$ is

$$(5.14)\quad {}_0\langle E,\theta',\phi'|T_s|E,\theta,\phi\rangle_0 \simeq \frac{|\underset{\sim}{k}|}{2}(\sin\theta\sin\theta')^{\frac{1}{2}} \lim_{|\underset{\sim}{k}'|\to|\underset{\sim}{k}|}\left\{\int \Psi^*_{st}(\underset{\sim}{x}|\underset{\sim}{k}')\left[-\nabla^2+V(\underset{\sim}{x})-k^2\right]\Psi_s(\underset{\sim}{x}|\underset{\sim}{k})d\underset{\sim}{x}\right\} + {}_0\langle E,\theta',\phi'|T_{st}|E,\theta,\phi\rangle_0$$

where the trial function $\Psi_{st}(\underset{\sim}{x}|\underset{\sim}{k})$ satisfies the boundary condition (5.12) with ${}_0\langle E,\theta',\phi'|T_s|E,\theta,\phi\rangle_0$ replaced by ${}_0\langle E,\theta',\phi'|T_{st}|E,\theta,\phi\rangle_0$.

6. Scattering of an electron by an atom

Let the eigenfunctions of the atom be denoted by $\chi(\underset{\sim}{y}|n)$ where $\underset{\sim}{y}$ designates the internal coordinates of the atom and n designates the state, i.e., n collectively denotes the eigenvalues of the energy, angular momentum, etc., of the atom. These eigenfunctions are to be so chosen that they satisfy the orthonormality and completeness relations

$$\int \chi^*(\underset{\sim}{y}|n)\,\chi(\underset{\sim}{y}|n')\,d\underset{\sim}{y} = \delta_{nn'} \tag{6.1}$$

$$\sum_n \chi^*(\underset{\sim}{y}|n)\,\chi(\underset{\sim}{y}'|n) = \delta(\underset{\sim}{y}-\underset{\sim}{y}'), \tag{6.2}$$

where $\delta_{nn'}$ denotes the product of Dirac and Kronecker δ's associated with the eigenvalues of energy and the degeneracy variables. In (6.2) the summation is to be interpreted as integration over continuous values.

We have

$$H_o = -\nabla^2_{\underset{\sim}{x}} + H^{(A)}_{\underset{\sim}{y}}, \tag{6.3}$$

$$H = H_o + V(\underset{\sim}{x}, \underset{\sim}{y}), \tag{6.4}$$

where $H^{(A)}_{\underset{\sim}{y}}$ is the Hamiltonian of the atom, and $V(\underset{\sim}{x},\underset{\sim}{y})$ is the interaction between the electron and the atom. The coordinates $\underset{\sim}{x}$ are the coordinates of the electron. We have then

$$\Psi_o(\underset{\sim}{x},\underset{\sim}{y}|\underset{\sim}{k},n) = \frac{1}{(2\pi)^{3/2}}\, e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}}\,\chi(\underset{\sim}{y}|n) \tag{6.5}$$

where $\underset{\sim}{x}$ represents the coordinates of the particles which is being scattered. The various Green's functions have the following forms:

$$G_E^{out}(\underset{\sim}{x},\underset{\sim}{y}|\underset{\sim}{x}',\underset{\sim}{y}') = -\frac{1}{4\pi}\sum_{n'} \frac{e^{i\sqrt{E-E_{n'}}\,|\underset{\sim}{x}-\underset{\sim}{x}'|}}{|\underset{\sim}{x}-\underset{\sim}{x}'|}\,\chi(\underset{\sim}{y}|n')\chi^*(\underset{\sim}{y}'|n'), \tag{6.6}$$

$$G_E^{in}(\underset{\sim}{x},\underset{\sim}{y}|\underset{\sim}{x}',\underset{\sim}{y}') = -\frac{1}{4\pi}\sum_{n'} \frac{e^{-i\sqrt{E-E_{n'}}\,|\underset{\sim}{x}-\underset{\sim}{x}'|}}{|\underset{\sim}{x}-\underset{\sim}{x}'|}\,\chi(\underset{\sim}{y}|n')\chi^*(\underset{\sim}{y}'|n'), \tag{6.7}$$

$$G_E^{s}(\underset{\sim}{x},\underset{\sim}{y}|\underset{\sim}{x}',\underset{\sim}{y}') = -\frac{1}{4\pi}\sum_{n'} \frac{\cos\sqrt{E-E_{n'}}\,|\underset{\sim}{x}-\underset{\sim}{x}'|}{|\underset{\sim}{x}-\underset{\sim}{x}'|}\,\chi(\underset{\sim}{y}|n')\chi^*(\underset{\sim}{y}'|n'). \tag{6.8}$$

In (6.6)-(6.8), E_n is the energy associated with the atomic state n.

The various eigenfunctions of the total Hamiltonian satisfy the integral equations

$$\Psi_{\pm}(\underset{\sim}{x},\underset{\sim}{y}|\underset{\sim}{k},n) = \frac{1}{(2\pi)^{3/2}}\, e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}}\,\chi(\underset{\sim}{y}|n)$$

$$(6.9) \qquad + \iint G_E^{\overset{\text{in}}{\text{out}}}(\underset{\sim}{x},\underset{\sim}{y}|\underset{\sim}{x}',\underset{\sim}{y}')V(\underset{\sim}{x}',\underset{\sim}{y}')\Psi_{\pm}(\underset{\sim}{x}',\underset{\sim}{y}'|\underset{\sim}{k},n)d\underset{\sim}{x}'d\underset{\sim}{y}',$$

$$\Psi_s(\underset{\sim}{x},\underset{\sim}{y}|\underset{\sim}{k},n) = \frac{1}{(2\pi)^{3/2}}\, e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}}\,\chi(\underset{\sim}{y}|n)$$

$$(6.10) \qquad + \iint G_E^{s}(\underset{\sim}{x},\underset{\sim}{y}|\underset{\sim}{x}',\underset{\sim}{y}')V(\underset{\sim}{x}',\underset{\sim}{y}')\Psi_s(\underset{\sim}{x}',\underset{\sim}{y}'|\underset{\sim}{k},n)d\underset{\sim}{x}'d\underset{\sim}{y}'.$$

The variable E occuring in (6.9) and (6.10) is given by

$$(6.11) \qquad E = |\underset{\sim}{k}|^2 + E_n .$$

In the general expression ${}_o\langle E,a|T_-|E,a'\rangle_o$ the variables a, a' are replaced by the quantum number giving the state of the atom and the polar angles of the momentum of the electron. This quantity can be obtained from the asymptotic form of $\Psi_-(\underset{\sim}{x},\underset{\sim}{y}|\underset{\sim}{k},n)$ as $|x| \to \infty$:

$$\lim_{|\underset{\sim}{x}|\to\infty} \Psi_-(\underset{\sim}{x},\underset{\sim}{y}|\underset{\sim}{k},n) = \frac{e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}}}{(2\pi)^{3/2}}\,\chi(\underset{\sim}{y}|n)$$

$$(6.12) \qquad - \left(\frac{2\pi}{|\underset{\sim}{k}|}\right)^{1/2}(\sin\theta\sin\theta')^{-1/2}\sum_{n'}\frac{e^{i|\underset{\sim}{k}_{n'}||\underset{\sim}{x}|}}{|\underset{\sim}{x}||\underset{\sim}{k}_{n'}|^{1/2}}\,\chi(\underset{\sim}{y}|n')$$

$${}_o\langle E,\theta',\phi',n'|T_-|E,\theta,\phi,n\rangle_o .$$

In (6.12) θ', ϕ' are the polar angles of $\underset{\sim}{x}$; θ, ϕ are those of $\underset{\sim}{k}$. Also $|\underset{\sim}{k}_{n'}|$ is defined by

$$(6.12a) \qquad |\underset{\sim}{k}_{n'}|^2 + E_{n'} = E = |\underset{\sim}{k}|^2 + E_n ,$$

$$(6.12b) \qquad \underset{\sim}{k}_n = \underset{\sim}{k} .$$

Likewise

$$\lim_{|\underset{\sim}{x}|\to\infty} \Psi_+(\underset{\sim}{x},\underset{\sim}{y}|\underset{\sim}{k},n) = \frac{e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}}}{(2\pi)^{3/2}}\chi(\underset{\sim}{y}|n) - \left(\frac{2\pi}{|\underset{\sim}{k}|}\right)^{\frac{1}{2}}(\sin\theta\sin\theta')^{-\frac{1}{2}}\sum_{n'}\frac{e^{-i|\underset{\sim}{k}_{n'}||\underset{\sim}{x}|}}{|\underset{\sim}{x}||\underset{\sim}{k}_{n'}|^{1/2}} \cdot \chi(\underset{\sim}{y}|n')\,{}_o\!< E,\pi-\theta',\pi+\phi',n'|T_+|E,\theta,\phi,n >_o \quad , \tag{6.13}$$

$$\lim_{|\underset{\sim}{x}|\to\infty} \Psi_s(\underset{\sim}{x},\underset{\sim}{y}|\underset{\sim}{k},n) = \frac{e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}}}{(2\pi)^{3/2}}\chi(\underset{\sim}{y}|n) - \left(\frac{\pi}{2|\underset{\sim}{k}|}\right)^{\frac{1}{2}}(\sin\theta\sin\theta')^{-\frac{1}{2}}\sum_{n'}\chi(\underset{\sim}{y}|n') \left\{\frac{e^{i|\underset{\sim}{k}_{n'}||\underset{\sim}{x}|}}{|\underset{\sim}{x}||\underset{\sim}{k}_{n'}|^{1/2}}\,{}_o\!< E,\theta',\phi',n'|T_s|E,\theta,\phi,n >_o + \frac{e^{-i|\underset{\sim}{k}_{n'}||\underset{\sim}{x}|}}{|x||\underset{\sim}{k}_{n'}|^{1/2}}\,{}_o\!< E,\pi-\theta',\pi+\phi',n'|T_s|E,\theta,\phi,n >_o\right\} , \tag{6.14}$$

where $\underset{\sim}{k}_{n'}$, θ',ϕ', $\underset{\sim}{k}$ are defined in (6.12a). The first of the two variational principles for this problem is

$${}_o\!< E,\theta',\phi',n'|T_-|E,\theta,\phi,n >_o \cong \frac{(|\underset{\sim}{k}||\underset{\sim}{k}'|\sin\theta\sin\theta')^{1/2}}{2} \cdot \lim_{E'\to E}\int \Psi^*_{+t}(\underset{\sim}{x},\underset{\sim}{y}|\underset{\sim}{k}',n')\left[H-|\underset{\sim}{k}|^2-E_n\right]\Psi_{-t}(\underset{\sim}{x},\underset{\sim}{y}|\underset{\sim}{k},n)d\underset{\sim}{x}d\underset{\sim}{y} + {}_o\!< E,\theta',\phi',n'|T_{-t}|E,\theta,\phi,n >_o \; . \tag{6.15}$$

In (6.15) we have

(6.15a)
$E = |\underset{\sim}{k}|^2 + E_n$;
$E' = |\underset{\sim}{k}'|^2 + E_{n'}$;
θ,ϕ are polar angles of $\underset{\sim}{k}$;
θ',ϕ' are polar angles of $\underset{\sim}{k}'$; when $E' = E$, then $|\underset{\sim}{k}'| = |\underset{\sim}{k}_{n'}|$, .

The functions $\Psi_{\pm t}$ have the asymptotic form (6.12) and (6.13) with $T_{\pm}$ replaced by $T_{\pm t}$. The second variational principle is

$$(6.16)\qquad {}_o\langle E,\theta',\phi',n'|T_s|E,\theta,\phi,n\rangle_o \simeq \frac{(|\underset{\sim}{k}||\underset{\sim}{k}'|\sin\theta\sin\theta')^{1/2}}{2} \cdot \lim_{E'\to E}\int \Psi^*_{st}(\underset{\sim}{x},\underset{\sim}{y}|\underset{\sim}{k}',n')\left[H-|\underset{\sim}{k}|^2-E_n\right]\Psi_{st}(\underset{\sim}{x},\underset{\sim}{y}|\underset{\sim}{k},n)\,d\underset{\sim}{x}\,d\underset{\sim}{y} + {}_o\langle E,\theta',\phi',n'|T_{st}|E,\theta,\phi,n\rangle_o ,$$

where Ψ_{st} has the form (6.14) but where T_s is replaced by T_{st}. Also, (6.15a) holds for (6.16).

7. Operators used in scattering theory

It will be convenient to prove the variational principle in terms of operators. Hence we shall summarize properties of operators useful in scattering theory. The details are given in [4].

As before, let us assume H_o has a purely continuous spectrum and $H = H_o + V$ has a spectrum which coincides with that of H_o; H may also have bound states. As before, the eigenvectors of H_o corresponding to the eigenvalues E and degeneracy variable a is given by $|E,a\rangle_o$. The corresponding eigenvector of H is designated by $|E,a\rangle$.

Let us introduce the operator U defined by

$$(7.1)\qquad |E,a\rangle = U|E,a\rangle_o .$$

All possible operators U satisfy the equations

$$(7.2)\qquad HU - UH_o = 0$$

or equivalently

$$(7.2a)\qquad U = L + \int \frac{P}{E-H_o}\, VU\,\delta(E-H_o)\,dE ,$$

where L is an arbitrary operator which commutes with H_o.

In (7.2) the operators $\frac{P}{E-H_o}$ and $\delta(E-H_o)$ appear. In accordance with the usual convention, we define any function $f(H_o)$ of the single operator H_o by

$$f(H_o)\,|E,a>_o = f(E)|E,a>_o \,. \tag{7.3}$$

The operators $\frac{P}{E-H_o}$ and $\delta(E-H_o)$ are also defined in this way, where the symbol P means that the Cauchy principal part of the integral is to be taken in integrals over the variable E. Some useful properties of $\frac{P}{E-H_o}$ and $\delta(E-H_o)$ are

$$(E-H_o)\,\frac{P}{E-H_o} = I, \tag{7.4}$$

$$(E-H_o)\,\delta(E-H_o) = 0, \tag{7.5}$$

$$\delta(E-H_o)f(E) = \delta(E-H_o)f(H_o) = f(H_o)\delta(E-H_o), \text{ for any function } f(E), \tag{7.6}$$

and

$$\int \delta(E-H_o)dE = I. \tag{7.7}$$

The incoming and outgoing eigenfunctions $|E,a>_\pm$ and the corresponding operators $U_\pm$ given by

$$|E,a>_\pm = U_\pm\,|E,a>_o \tag{7.8}$$

are defined by the requirements

$$\lim_{t\to-\infty} e^{iH_ot}\,e^{-iEt}\,|E,a>_- = |E,a>_o \,. \tag{7.9}$$

The equivalent requirement on U_- is

$$\lim_{t\to-\infty} e^{iH_ot}\,U_-e^{-iH_ot} = I, \tag{7.9a}$$

while for $|E,a>_+$, U_+ we have, also by definition,

$$(7.10)\qquad \lim_{t\to+\infty} e^{iH_0t} e^{-iEt} |E,a>_+ = |E,a>_0 ,$$

$$(7.10a)\qquad \lim_{t\to+\infty} e^{iH_0t} U_+ e^{-iH_0t} = I.$$

It can be shown that L must be so chosen that $U_\pm$ satisfies the equation

$$(7.11)\qquad U_\pm = I + \int \gamma_\pm(E-H_0)VU_\pm\delta(E-H_0)dE = I + \int \gamma_\pm(E-H_0)T_\pm\delta(E-H_0)dE ,$$

where

$$(7.12)\qquad T_\pm = VU_\pm$$

and

$$(7.13)\qquad \gamma_\pm(E-H_0) = \pm\, i\, \pi\delta(E-H_0) + \frac{P}{E-H_0} .$$

The scattering operator S and its inverse S^{-1} are defined by

$$(7.14)\qquad \lim_{t\to+\infty} e^{iH_0t} U_- e^{-iH_0t} = S,$$

$$(7.15)\qquad \lim_{t\to-\infty} e^{iH_0t} U_+ e^{-iH_0t} = S^{-1},$$

from which it can be shown that

$$(7.16)\qquad S = I - 2\pi i \int \delta(E-H_0)\, T_-\delta(E-H_0)dE$$

$$(7.16a)\qquad S^{-1} = I + 2\pi i \int \delta(E-H_0)T_+\delta(E-H_0)\, dE = S^* .$$

Equation (7.2a) for a general operator U can also be written

$$(7.17)\qquad U = M_\pm + \int \gamma_\pm\, (E-H_0)T\, \delta(E-H_0)\, dE ,$$

where

(7.18) $$T = VU,$$

(7.19) $$M_{\pm} = L \mp i\pi \int \delta(E-H_0)T\,\delta(E-H_0)\,dE.$$

In (7.6) the scattering operator was expressed in terms of T_- or equivalently U_-. It can also be expressed in terms of the general operator U, namely as

(7.20) $$S = M_+ M_-^{-1}.$$

The reactance operator is best motivated by choosing $M_{\pm}$ in such a way that S as given by (7.20) has a simple expression. Let us define the reactance operator K by the requirement that

(7.21) $$\begin{aligned} M_+ &= I - i\pi K \\ M_- &= I + i\pi K . \end{aligned}$$

Hence

(7.20a) $$S = (I - i\pi K)(I + i\pi K)^{-1}.$$

Since S is unitary, K must be Hermitian. Choosing $M_{\pm}$ in accordance with (7.21) means that we have specified L and hence U. We shall use the subscript s to designate the operator U and T so chosen.

From (7.19) we have

(7.22) $$M_+ + M_- = 2L, \qquad M_+ - M_- = -2i\pi \int \delta(E-H_0)T_s\delta(E-H_0)dE ,$$

while from (7.21)

(7.23) $$M_+ + M_- = 2I, \qquad M_+ - M_- = -2\pi iK.$$

Hence

$$(7.24) \qquad L = I, \qquad K = \int \delta(E-H_o)T_s\, \delta(E-H_o)\, dE\ .$$

To summarize:

$$(7.25) \qquad K = \int \delta(E-H_o)T_s\, \delta(E-H_o)dE,$$

where

$$(7.26) \qquad T_s = VU_s$$

$$(7.27) \qquad U_s = I + \int \frac{P}{E-H_o} VU_s\delta(E-H_o)dE = I + \int \frac{P}{E-H_o} T_s\delta(E-H_o)dE.$$

One could evaluate K, for example, by obtaining U_s by iteration, and substituting into (7.25). This procedure is an expansion in terms of Born approximations. It should be noted that $\frac{P}{E-H_o}$ is Hermitian. Hence $|E,a>_s = U_s|E,a>_o$ is characterized by a Hermitian Green's function.

The analogues to (7.9a) and (7.14) are

$$(7.28) \qquad \lim_{t\to-\infty} e^{iH_ot}U_se^{-iH_ot} = I + i\pi K = I + i\pi \int \delta(E-H_o)T_s\delta(E-H_o)dE,$$

$$(7.29) \qquad \lim_{t\to+\infty} e^{iH_ot}U_se^{-iH_ot} = I - i\pi K = I - i\pi \int \delta(E-H_o)T_s\delta(E-H_o)dE.$$

8. The variational principles in operator form

We shall now state the variational principles in operator form. The results can be translated immediately into the $\underset{\sim}{x}$-representations as given earlier. We shall prove the principles for the reactance operator. The proof of the variational principles for the scattering operator is similar and has already been given in [2].

Let us define the operator $R(T_{\pm t})$ by

$$(8.1) \qquad R(T_{\pm t}) = \lim_{\nu \to 0} \int \delta(E-\nu-H_o)W^{*}_{+t}(HW_{-t}-W_{-t}H_o)\delta(E-H_o)dE$$

$$+ \int \delta(E-H_o)T_{-t}\,\delta(E-H_o)dE,$$

where the asterisk means the Hermitian adjoint. The operator T_{-t} is a trial operator which approximates T_{-}, and W_{+t} and W_{-t} are trial operators which are to approximate U_{+} and U_{-} respectively and are chosen to satisfy the time-conditions

$$(8.2) \quad \begin{cases} \lim\limits_{t \to -\infty} e^{iH_o t} W_{-t}\, e^{-iH_o t} = I, \\ \\ \lim\limits_{t \to +\infty} e^{iH_o t} W_{-t}\, e^{-iH_o t} = I - 2\pi i \int \delta(E-H_o)T_{-t}\delta(E-H_o)dE \end{cases}$$

and

$$(8.3) \quad \begin{cases} \lim\limits_{t \to +\infty} e^{iH_o t} W_{+t}\, e^{-iH_o t} = I \\ \\ \lim\limits_{t \to -\infty} e^{iH_o t} W_{+t}\, e^{-iH_o t} = I + 2\pi i \int \delta(E-H_o)T_{+t}\delta(E-H_o)dE. \end{cases}$$

Note that W_{-t} and W_{+t} satisfy the same asymptotic time conditions as U_{-} and U_{+} [cf. (7.14), (7.15)] with $T_{\pm t}$ replaced by $T_{\pm}$.

Our theorem is that

$$(8.4) \qquad R(T_{\pm}) = \int \delta(E-H_o)T_{-}\delta(E-H_o)dE = \frac{i}{2\pi}\left[S-I\right].$$

Furthermore, the first variations of $R(T_{\pm t})$ due to variations of $T_{\pm t}$ about $T_{\pm}$ vanish. Hence

$$(8.5) \qquad \int \delta(E-H_o)\,T_{-}\,\delta(E-H_o) \cong R(T_{\pm t}), \qquad \text{when } T_{\pm t} = T_{\pm}.$$

The principle (8.4) reduces to (2.12) on writing

$$(8.6) \qquad \Psi_{\pm t}(\underset{\sim}{x}|E,a) = \langle \underset{\sim}{x}|W_{\pm t}|E,a \rangle_0 \ .$$

The conditions (8.2) and (8.3) which $W_{\pm t}$ are required to satisfy are completely equivalent to the conditions that $W_{\pm}$ be written as

$$(8.7) \qquad W_{\pm t} = I + \int \gamma_{\pm}(E-H_0)\, T_{\pm t}\, \delta(E-H_0)dE \ .$$

The boundary conditions which $\Psi_{\pm}(\underset{\sim}{x}|E,a)$ are required to satisfy in the various special cases above may be inferred from (8.7).

One may always think of the trial operators $T_{\pm t}$ as having the form

$$(8.8) \qquad T_{\pm t} = VU_{\pm t}$$

in analogy to (7.12); now $U_{\pm t}$ may be considered to be the trial operators. Then one can show

$$(8.9) \qquad R(T_{\pm t}) = \int \delta(E-H_0)A\, \delta(E-H_0)dE$$

where

$$(8.10) \qquad \begin{aligned} A = V + V\gamma_{-}(E-H_0)VU_{-t} + U^*_{+t}V\gamma_{-}(E-H_0)V - U^*_{+t}V\gamma_{-}(E-H_0)VU_{+t} \\ + U^*_{+t}V\gamma_{-}(E-H_0)V\gamma_{-}(E-H_0)VU_{-} \ . \end{aligned}$$

When (8.9) and (8.10) are used, the variational principle (8.5) takes the form (2.14) when we write

$$(8.11) \qquad \phi_{\pm t}(\underset{\sim}{x}|E,a) = \langle \underset{\sim}{x}|U_{\pm t}|E,a \rangle_0 \ .$$

We can obtain similar results for the reactance matrix. We shall now carry out the proofs for this case.

Let us define $\hat{R}(T_{st})$ as

$$(8.12) \qquad \hat{R}(T_{st}) = \lim_{\nu \to 0} \int \delta(E-\nu-H_o)W^*_{st}(HW_{st}-W_{st}H_o)\delta(E-H_o)dE$$
$$+ \int \delta(E-H_o)T_{st}\,\delta(E-H_o)dE,$$

where T_{st} approximates T_s, and W_{st} is required to satisfy the conditions

$$(8.13) \begin{cases} \lim\limits_{t \to -\infty} e^{iH_o t} W_{st} e^{-iH_o t} = I + i\pi \int \delta(E-H_o)T_{st}\delta(E-H_o)dE \\ \lim\limits_{t \to +\infty} e^{iH_o t} W_{st} e^{-iH_o t} = I - i\pi \int \delta(E-H_o)T_{st}\delta(E-H_o)dE. \end{cases}$$

Hence W_{st} has the same asymptotic form in time as U_s except that T_{st} in the former operator is replaced by T_s in the latter. The conditions on (8.13) are equivalent to

$$(8.14) \qquad W_{st} = I + \int \frac{P}{E-H_o} T_{st}\,\delta(E-H_o)dE ,$$

or

$$(8.14a) \qquad W_{st} = U_s + \int \frac{P}{E-H_o} \triangle T_s\,\delta(E-H_o)dE,$$

where

$$(8.14b) \qquad \triangle T_s = T_{st} - T_s .$$

We shall prove $\hat{R}(T_{st})$ is stationary for variations of T_{st} about T_s. Further we shall show

$$(8.15) \qquad \hat{R}(T_s) = K = \int \delta(E-H_o)\,T_s\,\delta(E-H_o)dE.$$

Hence

$$(8.16) \qquad K \cong \int \delta(E-H_o)T_s\delta(E-H_o)dE = \hat{R}(T_{st}), \quad \text{when } T_{st} \cong T_s .$$

Let us first prove (8.15). When $T_{st} = T_s$, then $\Delta T_s = 0$, and from (8.14a) $W = U_s$. But then $HW - WH_o = HU_s - U_sH_o = 0$ from (7.2). Hence the integral in (8.12) vanishes and

$$(8.17) \qquad \hat{R}(T_s) = \int \delta(E-H_o)T_s\delta(E-H_o)dE = K.$$

To show that $\hat{R}(T_{st})$ is stationary about $T_{st} = T_s$, let us write

$$(8.18) \qquad \Delta\hat{R} = \hat{R}(T_{st}) - \hat{R}(T_s) .$$

Then on using (8.14a) in (8.12) we have to the first order in ΔT_s

$$\begin{aligned} \Delta\hat{R} = \lim_{\nu\to 0} \Bigg\{ & \int \delta(E-\nu-H_o) \int \delta(E'-H_o)\, \Delta T_s^* \frac{P}{E'-H_o}\, dE'(HU_s-U_sH_o)\delta(E-H_o)dE \\ & + \int \delta(E-\nu-H_o)U_s^* \Bigg[H \int \frac{P}{E'-H_o}\, \Delta T_s\, \delta(E'-H_o)dE' \\ (8.19) \qquad & - \int \frac{P}{E'-H_o}\, \Delta T_s\delta(E'-H_o)dE'\, H_o\Bigg]\, \delta(E-H_o)dE \Bigg\} \\ & + \int \delta(E-H_o)\, \Delta T_s\, \delta(E-H_o)dE. \end{aligned}$$

The first integral vanishes as a consequence of (7.2). Let us denote by C the integral

$$\begin{aligned} C = \lim_{\nu\to 0} & \int \delta(E-\nu-H_o)U_s^* \Bigg[H \int \frac{P}{E'-H_o}\, \Delta T_s\, \delta(E'-H_o)dE' \\ (8.20) \qquad & - \int \frac{P}{E'-H_o}\, \Delta T_s\, \delta(E'-H_o)dE'H_o\Bigg]\, \delta(E-H_o)dE. \end{aligned}$$

On using

$$(8.21) \qquad \delta(\;\;'-H_o)\delta(E-H_o) = \delta(E'-E)\delta(E-H_o)$$

and

$$\delta(E-H_o)H_o = E\,\delta(E-H_o), \tag{8.22}$$

we have

$$C = \lim_{\nu\to 0}\int \delta(E-\nu-H_o)U_s^*(H-E)\,\frac{P}{E-H_o}\,\Delta T_s\,\delta(E-H_o)dE. \tag{8.23}$$

But

$$(H-E)\,\frac{P}{E-H_o} = (H_o+V-E)\,\frac{P}{E-H_o} = -I + V\,\frac{P}{E-H_o}\;.$$

Hence, since $U_s^*\,V = T_s^*$, we have

$$\begin{aligned} C = \lim_{\nu\to 0}\Big\{ &- \int \delta(E-\nu-H_o)U_s^*\,\Delta T_s\delta(E-H_o)dE \\ &+ \int \delta(E-\nu-H_o)T_s^*\,\frac{P}{E-H_o}\,\Delta T_s\,\delta(E-H_o)dE. \end{aligned} \tag{8.24}$$

But on using (7.27) for U_s^* in the first integral above and then using (8.21) and (8.22) to simplify the resulting expressions, we see

$$\begin{aligned} &\int \delta(E-\nu-H_o)\,U_s^*\,\Delta T_s\,\delta(E-H_o)dE \\ &= \int \delta(E-\nu-H_o)\,\Delta T_s\delta(E-H_o)dE + \int \delta(E-\nu-H_o)T_s^*\,\frac{P}{E-H_o}\,\Delta T_s\,\delta(E-H_o)dE. \end{aligned} \tag{8.25}$$

Thus

$$C = -\int \delta(E-H_o)\,\Delta T_s\,\delta(E-H_o)dE. \tag{8.26}$$

Hence, from (8.19), (8.20) and (8.22)

$$\Delta\hat{R} = 0 \tag{8.27}$$

to first order in ΔT_s, as desired.

The variational principle (8.16) reduces to (2.15) in terms of the $\underset{\sim}{x}$-representation when we write

(8.28) $$\Psi_{st}(\underset{\sim}{x}|E,a) = <\underset{\sim}{x}|W_{st}|E,a>_o \;.$$

The initial and final conditions (8.11) lead to the given boundary conditions required on $\Psi_{st}(\underset{\sim}{x}|E,a)$ for the various special cases.

We can get another form for the variational principle for the reactance operator by substituting (8.14) into (8.12). We have

(8.29) $$\begin{aligned}\hat{R}(T_{st}) = \lim_{\nu\to 0} \Bigg\{ & \int \delta(E-H_o-\nu)(H-H_o)\delta(E-H_o)dE \\ & + \int \delta(E-\nu-H_o)\left[\int \delta(E'-H_o)T^*_{st}\,\frac{P}{E'-H_o}\,dE'\right](H-H_o)\delta(E-H_o)dE \\ & + \int \delta(E-\nu-H_o)\Bigg[H\int \frac{P}{E'-H_o}\,T_{st}\delta(E'-H_o)dE' \\ & \qquad - \int \frac{P}{E'-H_o}\,T_{st}\delta(E'-H_o)dE'H_o\Bigg]\,\delta(E-H_o)dE \\ & + \int \delta(E-\nu-H_o)\left[\int \delta(E'-H_o)T^*_{st}\,\frac{P}{E'-H_o}\,dE'\right] \\ & \qquad \cdot \Bigg[H\int \frac{P}{E''-H_o}\,T_{st}\,\delta(E''-H_o)dE'' \\ & \qquad - \int \frac{P}{E''-H_o}\,T_{st}\,\delta(E''-H_o)dE''H_o\Bigg]\delta(E-H_o)dE \Bigg\} \\ & + \int \delta(E-H_o)\,T_{st}\,\delta(E-H_o)dE.\end{aligned}$$

Noting that $H - H_o = V$ and using (8.21) and (8.22), and writing, as we may

(8.30) $$T_{st} = VU_{st} \;,$$

we obtain finally,

(8.31) $$\hat{R}(T_{st}) = \int \delta(E-H_o)\,\hat{A}\,\delta(E-H_o)\,dE,$$

where

$$(8.32)\quad \begin{aligned}\hat{A} = \; & V + V \frac{P}{E-H_o} VU_{st} + U_{st}^{*} V \frac{P}{E-H_o} V - U_{st}^{*} V \frac{P}{E-H_o} VU_{st} \\ & + U_{st}^{*} V \frac{P}{E-H_o} V \frac{P}{E-H_o} VU_{st} \; .\end{aligned}$$

Since $\frac{P}{E-H_o}$ is Hermitian, $\hat{A}$ and $\hat{R}$ are also Hermitian for any trial operator U_{st}. Hence for any trial operator U_{st}, or equivalently T_{st}, the reactance operator K will be approximated by the Hermitian operator $\hat{R}$.

Using $\hat{R}$ in the form (8.31) and $\hat{A}$ given by (8.32), we obtain the variational principle in the form (2.16) when we write

$$(8.33)\qquad \phi_{st}(\underset{\sim}{x}|E,a) = <\underset{\sim}{x}|U_{st}|E,a>_o .$$

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